

Perrhenate and Pertchnetate Behavior on Iron and Sulfur-Bearing Compounds.

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Investigations on the behavior of the radioactive element technetium frequently use a stable isotope of rhenium as an analogue. This is justified by citing the elements' similar radii and major oxidation states of +7 and +4. However, at least one study [1] has shown this analogy to be imperfect. Therefore, one goal of our study is to compare the adsorption behavior of perrhenate and pertchnetate (the major forms of Re and Tc in natural waters) on a number of different mineral surfaces.

Quantum mechanical calculations were performed on the adsorption of these two anions on a series of iron oxides and sulfides. With these calculations, we gain insight into any differences between the anions' adsorption behavior, including geometry, adsorption energies, and electronic structure such as density of states and orbital shapes and energies at the adsorption site. Differences between interactions on terraces and step edges, the effects of co-adsorbates such as Na⁺ or H⁺, and possible reduction mechanisms are also explored. The influence of water was calculated using homogeneous dielectric fluids and explicit water molecules.

As a complement to the calculations, batch sorption tests are in progress involving ReO₄⁻/TcO₄⁻ solution in contact with Fe metal, 10% Fe-doped hydroxyapatite, goethite, hematite, magnetite, pyrite, galena, and sphalerite.

References

[1] Wharton, M.J., Atkins, B., Charnock, J.M., Livens, F.R.; Patrick, R.A.D., and Collison, D. (2000) *Appl. Geochem* **15**, 374-354.

*This work is supported through the DOE OCRWM Office of Science and Technology and International (OS&T)